SUNDIALS: Suite of Nonlinear and Differential/Algebraic Equation Solvers

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and

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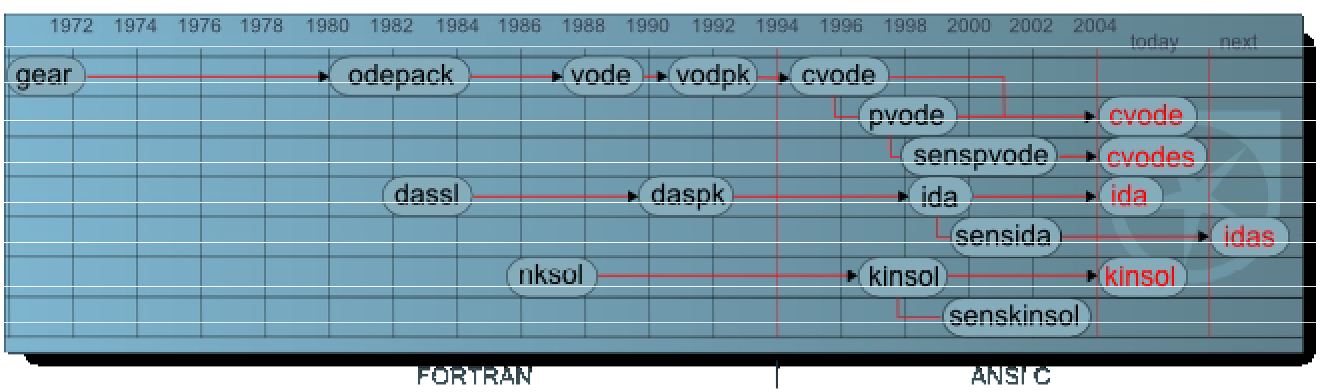
Outline

- SUNDIALS Overview
- ODE and DAE integration
  - Initial value problems
  - Implicit integration methods
- Nonlinear Systems
  - Newton’s method and inexact Newton’s method
  - Preconditioning
- Sensitivity analysis
  - Definitions, applications, methods
  - Forward sensitivity analysis
  - Adjoint sensitivity analysis
- SUNDIALS: usage, applications, and availability

LLNL has a long history of R&D in ODE/DAE methods and software

- **Fortran solvers written at LLNL:**
  - —VODE: stiff/nonstiff ODE systems, with direct linear solvers
  - —VODPK: with Krylov linear solver (GMRES)
  - —NKSOL: Newton-Krylov solver - nonlinear algebraic systems
  - —DASPK: DAE system solver (from DASSL)
- **Recent focus has been on parallel solution of large-scale problems and on sensitivity analysis**



Push to solve large, parallel systems motivated rewrites in C

- **CVODE:** rewrite of VODE/VODEPK [Cohen, Hindmarsh, 94]
- **PVODE:** parallel CVODE [Byrne and Hindmarsh, 98]
- **KINSOL:** rewrite of NKSOL [Taylor and Hindmarsh, 98]
- **IDA:** rewrite of DASPK [Hindmarsh and Taylor, 99]
- **Sensitivity variants: SensPVODE, SensIDA, SensKINSOL [Brown, Grant, Hindmarsh, Lee, 00-01]**
- **New sensitivity-capable solvers:**
  - **CVODES [Hindmarsh and Serban, 02]**
  - **IDAS – in development**

- **Organized into a single suite, SUNDIALS, including CVODE and CVODES, IDA, KINSOL, and soon IDAS**

The SUNDIALS package offers Newton solvers, time integration, and sensitivity solvers

- **CVODE: implicit ODE solver, $y' = f(y, t)$**
  - Variable-order, variable step BDF (stiff) or implicit Adams (nonstiff)
  - Nonlinear systems solved by Newton or functional iteration
  - Linear systems by direct (dense or band) or iterative solvers
- **IDA: implicit DAE solver, $F(t, y, y') = 0$**
  - Variable-order, variable step BDF
  - Nonlinear system solved by Newton iteration
  - Linear systems by direct (dense or band) or iterative solvers
- **KINSOL: Newton solver, $F(u) = 0$**
  - Inexact and Modified (with dense solve) Newton
  - Linear systems by iterative or dense direct solvers
- **CVODES: sensitivity-capable (forward & adjoint) CVODE**
- **IDAS: sensitivity-capable (forward & adjoint) IDA**
- **Iterative linear Krylov solvers: GMRES, BiCGStab, TFQMR**

SUNDIALS was designed to easily interface with legacy codes

- **Philosophy: *Keep codes simple to use***
- **Written in C**
  - **Fortran interfaces: fcvode, fida, and fkinsol**
  - **Matlab interfaces: sundialsTB (cvodes and kinsol)**
- **Written in a data structure neutral manner**
  - **No specific assumptions about data**
  - **Application-specific data representations can be used**
- **Modular implementation**
  - **Vector modules**
  - **Linear solver modules**
- **Require minimal problem information, but offer user control over most parameters**

Initial value problems (IVPs) come in the form of ODEs and DAEs

- The general form of an IVP is given by

$$F(\dot{x}, x) = 0$$
$$x(t_0) = x_0$$

- If $\partial F / \partial \dot{x}$ is invertible, we solve for $\dot{x}$ to obtain an ordinary differential equation (ODE)
- Else, the IVP is a differential algebraic equation (DAE)

- A DAE has differentiation index *i* if *i* is the minimal number of analytical differentiations needed to extract an explicit ODE

Stiffness of an equation can significantly impact whether implicit methods are needed

- **(Ascher and Petzold, 1998): If the system has widely varying time scales, and the phenomena that change on fast scales are *stable*, then the problem is stiff**
- **Stiffness depends on**
  - **Jacobian eigenvalues, λ_j**
  - **System dimension**
  - **Accuracy requirements**
  - **Length of simulation**
- **In general a problem is stiff on $[t_0, t_1]$ if**

$$\boxed{(t_1 - t_0)\min_j \Re(\lambda_j) << -1}$$

Dalquist test problem shows impact of stability on step sizes for explicit and implicit methods

Dalquist test equation: $\dot{y} = \lambda y, \quad y_0 = 1$

Exact solution: $y(t_n) = y_0 e^{\lambda t_n}$

Absolute stability requirement

$$|y_n| \leq |y_{n-1}|, \quad n = 1,2,\ldots$$

Reason: If Re(λ)<0, then $|y(t_n)|$ decays exponentially, and we cannot tolerate growth in y_n

Region of absolute stability: $S = \{z \in C; |R(z)| \leq 1\}$

where an integrator can be written as $y_n = R(z) y_{n-1}$, with time step $z = h\lambda$

Forward and backward Euler show different stability restrictions

- **Forward Euler:** $y_n = y_{n-1} + h(\lambda y_{n-1}) \Rightarrow R(z) = 1 + h\lambda$

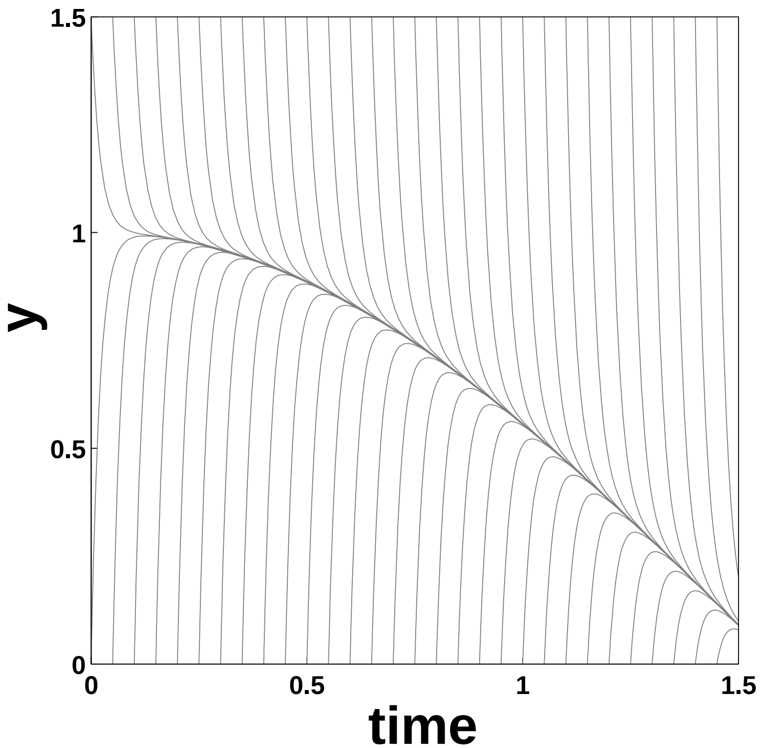
So, if λ < 0, FE has the step size restriction: $h \le \frac{2}{-\lambda}$

- **Backward Euler:** $y_n = y_{n-1} + h(\lambda y_n) \Rightarrow R(z) = \frac{1}{1 - h\lambda}$

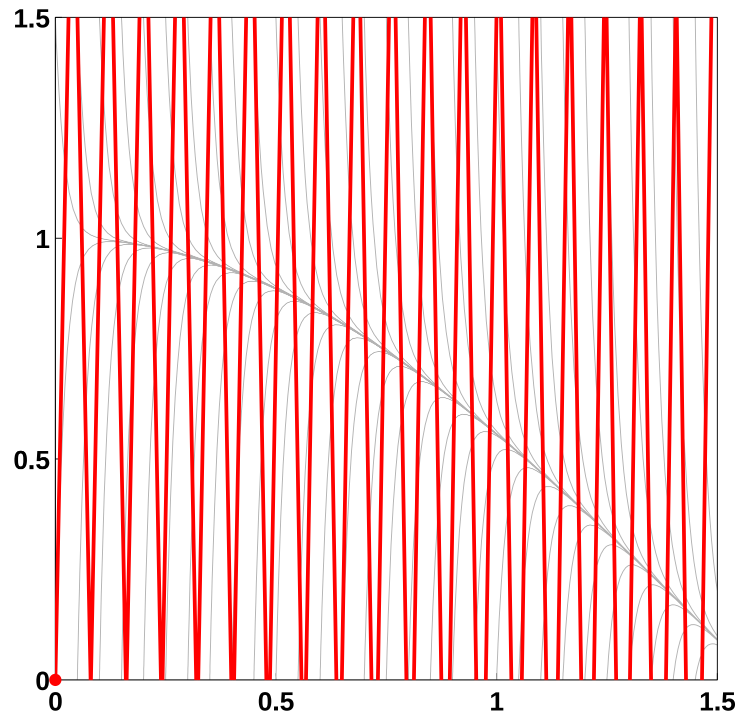
So, if λ < 0, BE has the step size restriction: $h > 0$

Curtiss and Hirchfelder example

$$\dot{y} = -50\left(y - \cos(t)\right) \quad \lambda = -50$$



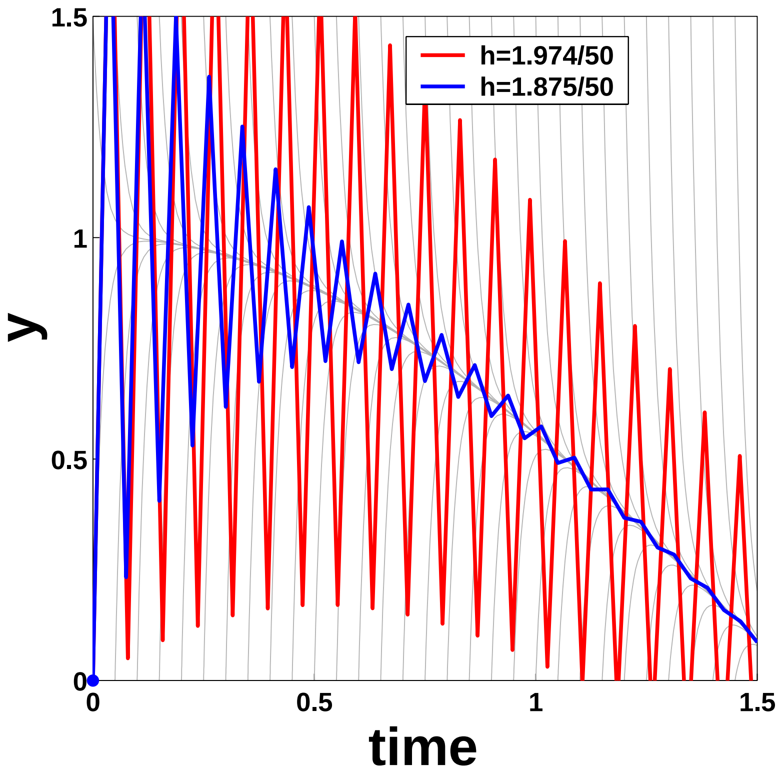
Solution curves



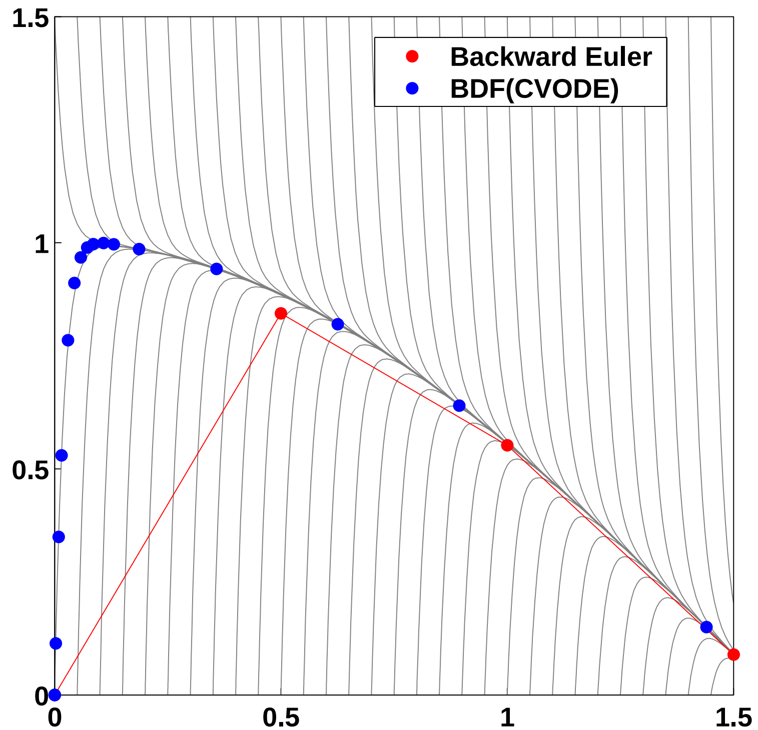
Forward Euler
h=2.01/50

Curtiss and Hirchfelder example

$$\dot{y} = -50(y - cos(t)) \quad \lambda = -50$$



Forward Euler



Implicit schemes
h=0.5 for BE

SUNDIALS has implementations of Linear Multistep Methods (LMM)

General form of LMM: $$\sum_{i=0}^{K_1} \alpha_{n,i} y_{n-i} + h_n \sum_{i=0}^{K_2} \beta_{n,i} \dot{y}_{n-i} = 0$$

- **Two methods:**
  - Adams-Moulton (nonstiff); $K_1 = 1$, $K_2 = k$, $k = 1,\ldots,12$
  - BDF (stiff); $K_1 = k$, $K_2 = 0$, $k = 1,\ldots,5$

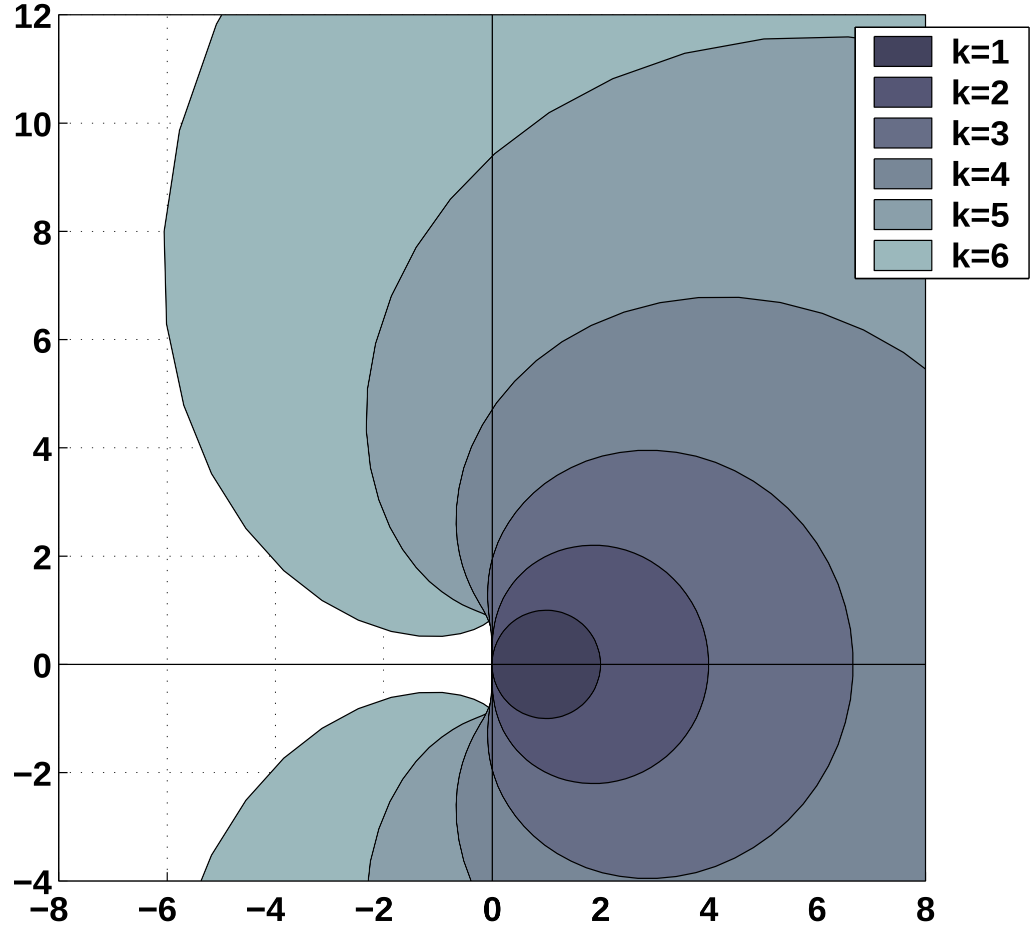
- **Nonlinear systems (BDF)**
  - ODE:

    $\dot{y} = f(y)$ $$G(y_n) \equiv y_n - \beta_0 h_n f(y_n) - \sum_{i=1}^{k} \alpha_{n,i} y_{n-i} = 0$$
  - DAE:

    $F(\dot{y}, y) = 0$ $$G(y_n) \equiv F\left((\beta_0 h_n)^{-1} \sum_{i=1}^{k} \alpha_{n,i} y_{n-i}, y_n \right) = 0$$

Stability is very restricted for higher orders of BDF methods

$$y_n - \beta_0 h_n \dot{y}_n = \sum_{i=1}^{k} \alpha_{n,i} y_{n-i}$$



CVODE solves y'=f(t,y)

- Variable order and variable step size methods:
  - BDF (backward differentiation formulas) for stiff systems
  - Implicit Adams for nonstiff systems
- (Stiff case) Solves time step for the system $\dot{y} = f(t, y)$
  - applies an explicit predictor to give $y_{n(0)}$

$$y_{n(0)} = \sum_{j=1}^{q} \alpha_j^p y_{n-j} + \Delta t \beta_1^p \dot{y}_{n-1}$$

  - applies an implicit corrector with $y_{n(0)}$ as the initial guess

$$y_n = \sum_{j=1}^{q} \alpha_j y_{n-j} + \Delta t \beta_0 f_n(y_n)$$

Time steps are chosen to minimize the local truncation error

- Time steps are chosen by:
  - Estimate the error: $E(\Delta t) = C(y_n - y_{n(0)})$
    - Accept step if $||E(\Delta t)||_{WRMS} < 1$
    - Reject step otherwise
  - Estimate error at the next step, $\Delta t'$, as

$$E(\Delta t') \approx (\Delta t' / \Delta t)^{q+1} E(\Delta t)$$

  - Choose next step so that $||E(\Delta t')||_{WRMS} < 1$
- Choose method order by:
  - Estimate error for next higher and lower orders
  - Choose the order that gives the largest time step meeting the error condition

Computations weighted so no component disproportionally impacts convergence

- **An absolute tolerance is specified for each solution component, $ATOL^i$**
- **A relative tolerance is specified for all solution components, RTOL**
- **Norm calculations are weighted by:**

$$ewt^i = \frac{1}{RTOL \cdot |y^i| + ATOL^i} \qquad \|y\|_{WRMS} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(ewt^i \cdot y^i\right)^2}$$

- **Bound time integration error with:**

$$\|y_n - y_{n(0)}\| < \tfrac{1}{6}$$

The 1/6 factor tries to account for estimation errors

Nonlinear system will require nonlinear solves

- Use predicted value as the initial iterate for the nonlinear solver
- Nonstiff systems: Functional iteration

$$y_{n(m+1)} = \beta_0 h_n f\left(y_{n(m)}\right)$$

- Stiff systems: Newton iteration

$$M\left(y_{n(m+1)} - y_{n(m)}\right) = -G\left(y_{n(m)}\right)$$

  — ODE: $M \approx I - \gamma\, \partial f / \partial y\,, \quad \gamma = \beta_0 h_n$

  — DAE: $M \approx \partial F / \partial y + \gamma\, \partial F / \partial \dot{y}\,, \quad \gamma = 1/\left(\beta_0 h_n\right)$

SUNDIALS provides many options for linear solvers

- **Iterative linear solvers**
  - **Result in inexact Newton solver**
  - **Scaled preconditioned solvers: GMRES, Bi-CGStab, TFQMR**
  - **Only require matrix-vector products**
  - **Require preconditioner for the Newton matrix, *M***
- **Jacobian information (matrix or matrix-vector product) can be supplied by the user or estimated with finite difference quotients**
- **Two options require serial environments and some pre-defined structure to the data**
  - **Direct dense**
  - **Direct band**

An inexact Newton-Krylov method can be used to solve the implicit systems

- Krylov iterative method finds linear system solution in Krylov subspace: $K(J,r) = \{r, \quad Jr, \quad J^2r, \quad \ldots\}$
- Only require matrix-vector products
- Difference approximations to the matrix-vector product are used,

$$J(x)v \approx \frac{F(x+\theta v) - F(x)}{\theta}$$

- Matrix entries need never be formed, and memory savings can be used for a better preconditioner

IDA solves $F(t, y, y') = 0$

- C rewrite of DASPK [Brown, Hindmarsh, Petzold]
- Variable order / variable coefficient form of BDF
- Targets: implicit ODEs, index-1 DAEs, and Hessenberg index-2 DAEs
- Optional routine solves for consistent values of y_0 and y_0'
  - Semi-explicit index-1 DAEs, differential components known, algebraic unknown OR all of y_0' specified, y_0 unknown
- Nonlinear systems solved by Newton-Krylov method

- Optional constraints: $y^i > 0$, $y^i < 0$, $y^i \geq 0$, $y^i \leq 0$

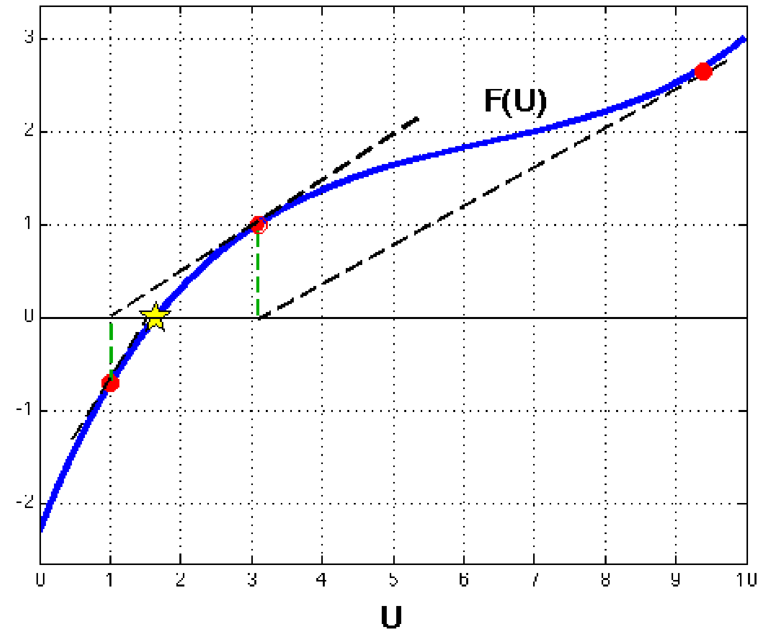
KINSOL solves $F(u) = 0$

- C rewrite of Fortran NKSOL (Brown and Saad)
- Inexact Newton solver: solves $J\,\Delta u^n = -F(u^n)$ approximately
- Modified Newton (with direct solves) – this freezes the Newton matrix over a number of iterations
- Krylov solver: scaled preconditioned GMRES, TFQMR, Bi-CGStab
  - Optional restarts for GMRES
  - Preconditioning on the right: $(J\,P^{-1})(Ps) = -F$
- Direct solvers: dense and band (serial & special structure)
- Optional constraints: $u_i > 0$, $u_i < 0$, $u_i \geq 0$ or $u_i \leq 0$
- Can scale equations and/or unknowns
- Dynamic linear tolerance selection

An inexact Newton's method is used to solve the nonlinear problem

1. Starting with x^0, want x^* such that $F(x^*) = 0$
2. Repeat for each k until $\left\| F(x^{k+1}) \right\| \leq tol$
   a. Solve (approximately) $J(x^k)s^k = -F(x^k)$
   b. Update, $x^{k+1} = x^k + \lambda s^k$

- tol may be chosen adaptively based on accuracy requirements
- λ is a search parameter
- ||.|| is a weighted L-2 norm



Linear stopping tolerances must be chosen to prevent “oversolves”

The linear system is solved to a given tolerance:

$$\left\|\mathbf{F}(\mathbf{x}^{\mathbf{k}}) + \mathbf{J}(\mathbf{x}^{\mathbf{k}})\mathbf{s}^{\mathbf{k+1}}\right\| \le \eta^{\mathbf{k}} \left\|\mathbf{F}(\mathbf{x}^{\mathbf{k}})\right\|$$

- **Newton method assumes a linear model**
  - **Bad approximation far from solution, loose tol.**
  - **Good approximation close to solution, tight tol.**
- **Eisenstat and Walker (SISC 96)**
  - **Choice 1** $\eta^k = \left\| \|F^k\| - \|F^{k-1} - J^{k-1}s^{k-1}\| \right\| \Big/ \|F^{k-1}\|$
  - **Choice 2** $\eta^{\mathbf{k}} = \mathbf{0.9}\left(\|\mathbf{F}^{(\mathbf{k})}\| \big/ \|\mathbf{F}^{(\mathbf{k-1})}\|\right)^{2}$
- **ODE literature** $\eta^k = \mathbf{0.05}$

Inexact methods maintain the fast rate of convergence of Newton's method

- Convergence of Newton's method is *q-quadratic* locally, for some constant C

$$\left\| \mathbf{x}^{k+1} - \mathbf{x}^{*} \right\| \leq C \left\| \mathbf{x}^{k} - \mathbf{x}^{*} \right\|^{2}$$

- Convergence of an inexact Newton method is
  - *q-linear* if, η^{k} is constant in *k*
  - *q-super-linear* if, $\lim_{k \to \infty} \eta^{k} = 0$
  - *q-quadratic* if for some constant C

$$\left\| F(x^{k}) + J(x^{k}) s^{k+1} \right\| \leq C \left\| F(x^{k}) \right\|^{2}$$

- Eisenstat and Walker methods are *q-quadratic*

Line-search globalization for Newton's method can enhance robustness

- User can select:
  - Inexact Newton
  - Inexact Newton with line search
- Line searches can provide more flexibility in the initial guess (larger time steps)
- Take, $x^{k+1} = x^k + \lambda s^{k+1}$, for λ chosen appropriately (to satisfy the Goldstein-Armijo conditions):
  - sufficient decrease in F relative to the step length
  - minimum step length relative to the initial rate of decrease
  - full Newton step when close to the solution

Preconditioning is essential for large problems as Krylov methods can stagnate

- **Preconditioner P must approximate Newton matrix, yet be reasonably efficient to evaluate and solve.**
- **Typical P (for time-dep. problem) is** $I - \gamma\tilde{J}, \quad \tilde{J} \approx J$
- **The user must supply two routines for treatment of P:**
  - **Setup: evaluate and preprocess P (infrequently)**
  - **Solve: solve systems Px=b (frequently)**
- **User can save and reuse approximation to J, as directed by the solver**
- **SUNDIALS offers hooks for user-supplied preconditioning**

Sensitivity Analysis

- **Sensitivity Analysis (SA) is the study of how the variation in the output of a model (numerical or otherwise) can be apportioned, qualitatively or quantitatively, to different sources of variation in inputs.**
- **Applications:**
  - **Model evaluation (most and/or least influential parameters), Model reduction, Data assimilation, Uncertainty quantification, Optimization (parameter estimation, design optimization, optimal control, …)**
- **Approaches:**
  - **Forward sensitivity analysis**
  - **Adjoint sensitivity analysis**

Sensitivity Analysis Approaches

Parameter dependent system

$$\begin{cases} F(x,\dot{x},t,p)=0 \\ x(0)=x_0(p) \end{cases}$$

FSA	ASA
$\begin{cases} F_{\dot{x}}\dot{s}_i + F_x s_i + F_{p_i} = 0 \\ s_i(0) = dx_0/dp_i \end{cases}, \quad i=1,\ldots,N_p$	$\begin{cases} (\lambda^* F_{\dot{x}})' - \lambda^* F_x = -g_x \\ \lambda^* F_{\dot{x}} x_p = \ldots \quad \text{at } t=T \end{cases}$
$g(t,x,p)$ $\frac{dg}{dp} = g_x s + g_p$	$G(x,p) = \int_0^T g(t,x,p)dt$ $\frac{dG}{dp} = \int_0^T (g_p - \lambda^* F_p)dt - \left(\lambda^* F_{\dot{x}} x_p\right)\Big|_0^T$
Computational cost: **$(1+N_p)N_x$ increases with N_p**	**Computational cost:** **$(1+N_g)N_x$ increases with N_g**

FSA - Methods

- **Staggered Direct Method:** On each time step, converge Newton iteration for state variables, then solve linear sensitivity system
  - Requires formation and storage of Jacobian matrices, Not matrix-free, Errors in finite-difference Jacobians lead to errors in sensitivities
- ✓ **Simultaneous Corrector Method:** On each time step, solve the nonlinear system simultaneously for solution and sensitivity variables
  - Block-diagonal approximation of the combined system Jacobian, Requires formation of sensitivity R.H.S. at every iteration
- ✓ **Staggered Corrector Method:** On each time step, converge Newton for state variables, then iterate to solve sensitivity system
  - With Krylov

FSA – Generation of the sensitivity system

- **Analytical**
- **Automatic differentiation**
  - **ADIFOR, ADIC, ADOLC**
  - **complex-step derivatives**
- **Directional derivative approximation**

CVODES case

$$\dot{x} = f(t,x,p)$$

$$\dot{s}_i = \frac{\partial f}{\partial x} s_i + \frac{\partial f}{\partial p_i}$$

$$\frac{\partial f}{\partial x} s_i \approx \frac{f(t, x+\sigma_x s_i, p) - f(t, x-\sigma_x s_i, p)}{2\sigma_x}$$

$$\frac{\partial f}{\partial p_i} \approx \frac{f(t, x, p+\sigma_i e_i) - f(t, x, p-\sigma_i e_i)}{2\sigma_i}$$

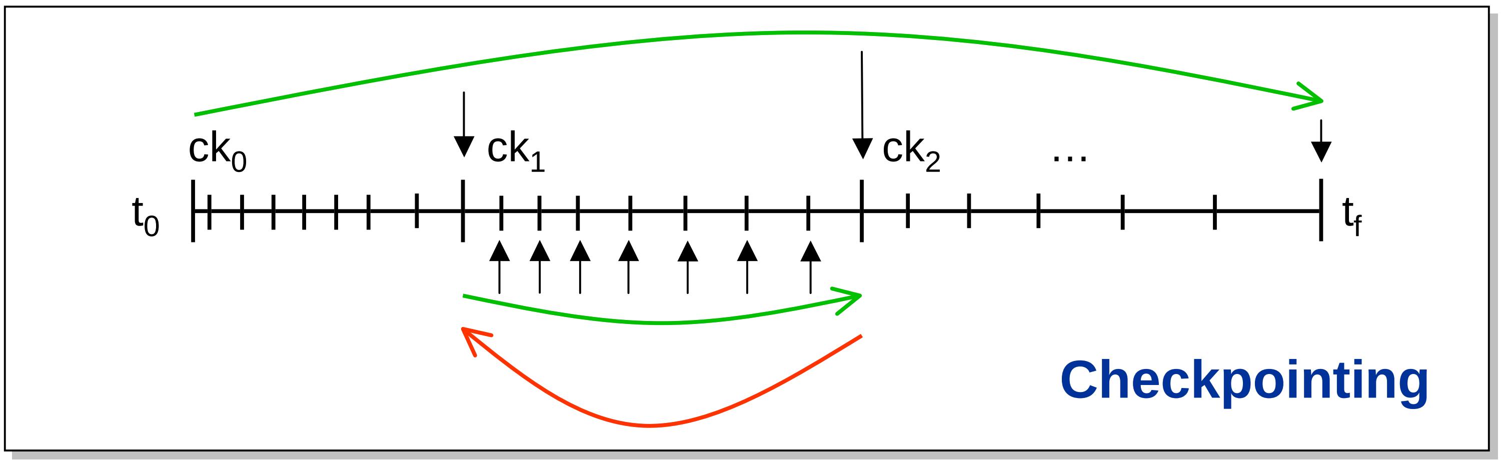
$$\begin{cases} \sigma_i = |\bar{p}_i| \sqrt{\max(rtol, \varepsilon)} \\ \sigma_x = \dfrac{1}{\max\left(1/\sigma_i, \|s_i\|_{WRMS} / |\bar{p}_i|\right)} \end{cases}$$

or

$$\frac{\partial f}{\partial x} s_i + \frac{\partial f}{\partial p_i} \approx \frac{f(t, x+\sigma s_i, p+\sigma e_i) - f(t, x-\sigma s_i, p-\sigma e_i)}{2\sigma} \qquad \sigma = \min(\sigma_i, \sigma_x)$$

ASA – Implementation

- **Solution of the forward problem is required for the adjoint problem → need predictable and compact storage of solution values for the solution of the adjoint system**



  - **Cubic Hermite or variable-degree polynomial interpolation**
  - **Simulations are reproducible from each checkpoint**
  - **Force Jacobian evaluation at checkpoints to avoid storing it**
  - **Store solution and first derivative**
  - **Computational cost: 2 forward and 1 backward integrations**

ASA – Generation of the sensitivity system

- **Analytical**
  - Tedious
  - For PDEs: in general, adjoint and discretization operators do NOT commute
- **Automatic differentiation**
  - Certainly the most attractive alternative
  - Reverse AD tools not as mature as forward AD tools
- **Finite difference approximation**
  - NOT an option (computational cost equivalent to FSA!)

The SUNDIALS vector module is generic

- Data vector structures can be user-supplied
- The generic NVECTOR module defines:
  - A `content` structure (void *)
  - An ops structure – pointers to actual vector operations supplied by a vector definition
- Each implementation of NVECTOR defines:
  - Content structure specifying the actual vector data and any information needed to make new vectors (problem or grid data)
  - Implemented vector operations
  - Routines to clone vectors
- Note that all parallelism (if needed) resides in reduction operations: dot products, norms, mins, etc.

SUNDIALS provides serial and parallel NVECTOR implementations

- Use is, of course, optional
- Vectors are laid out as an array of doubles (or floats)
- Appropriate lengths (local, global) are specified
- Operations are fast since stride is always 1
- All vector operations are provided for both serial and parallel cases
- For the parallel vector, MPI is used for global reductions

- These serve as good templates for creating a user-supplied vector structure around a user's own existing structures

SUNDIALS provides Fortran interfaces

- CVODE, IDA, and KINSOL
- Cross-language calls go in both directions:
- Fortran user code ←→ interfaces ←→ CVODE/KINSOL/IDA

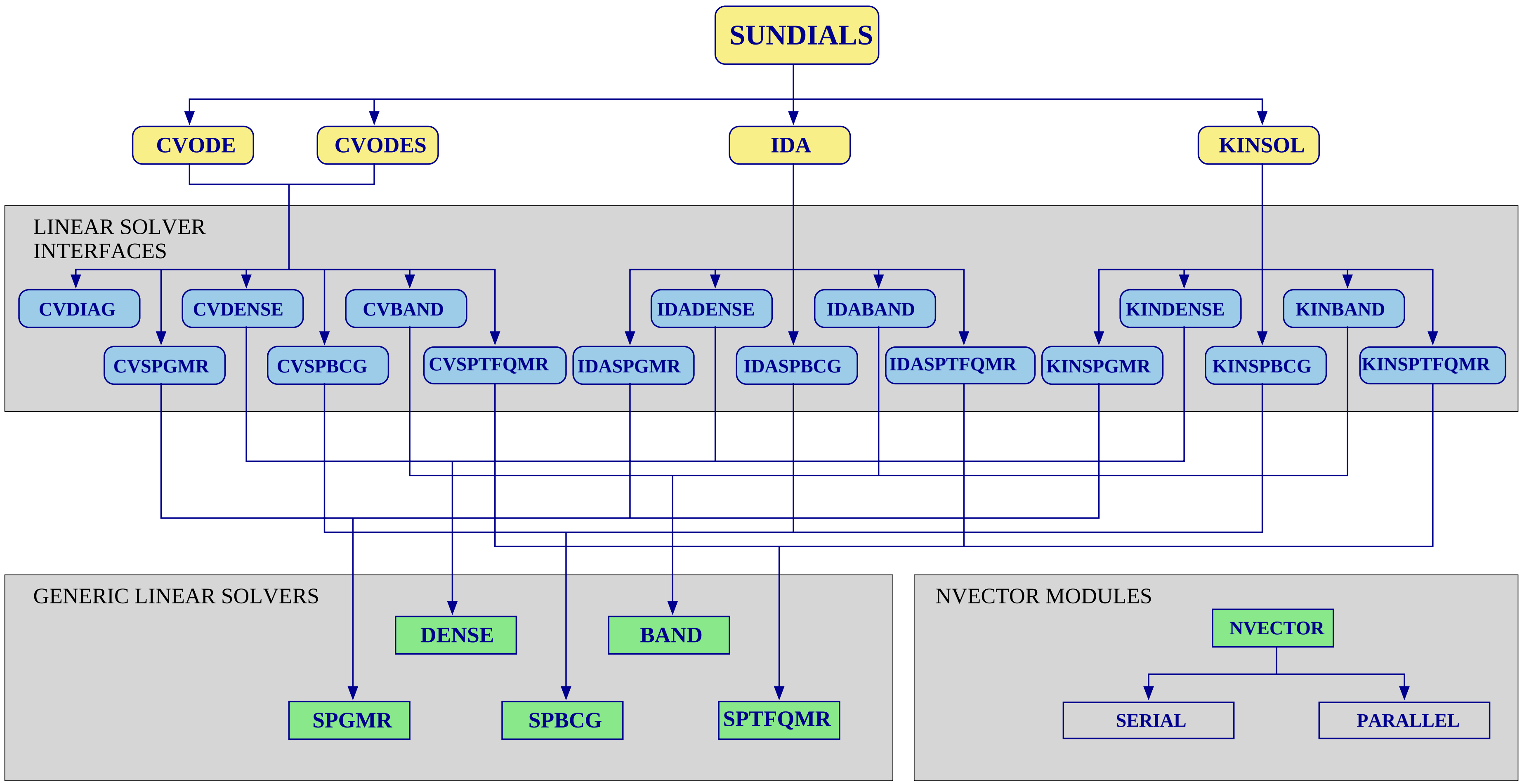
- Fortran main → interfaces to solver routines
- Solver routines → interface to user’s problem-defining routine and preconditioning routines

- For portability, all user routines have fixed names
- Examples are provided

SUNDIALS provides Matlab interfaces

- CVODES, KINSOL, and (next release) IDA
- The core of each interface is a single MEX file which interfaces to solver-specific user-callable functions
- Guiding design philosophy: make interfaces equally familiar to both SUNDIALS and Matlab users
  - all user-provided functions are Matlab m-files
  - all user-callable functions have the same names as the corresponding C functions
  - unlike the Matlab ODE solvers, we provide the more flexible SUNDIALS approach in which the 'Solve' function only returns the solution at the next requested output time.
- Includes complete documentation (including through the Matlab help system) and several examples

Structure of SUNDIALS



SUNDIALS code usage is similar across the suite

- Have a series of Set/Get routines to set options
- For CVODE with parallel vector implementation:

```
#include "cvode.h"
#include "cvode_spgmr.h"
#include "nvector_*.h"

y = N_VNew_*(n,…);
cvmem = CVodeCreate(CV_BDF,CV_NEWTON);
flag = CVodeSet*(…);
flag = CVodeMalloc(cvmem,rhs,t0,y,…);
flag = CVSpgmr(cvmem,…);
for(tout = …) {
   flag = CVode(cvmem, …,y,…);  }

NV_Destroy(y);
CVodeFree(&cvmem);
```

Forward Sensitivity Analysis in SUNDIALS

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```
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#include "cvodes_spgmr.h"
#include "nvector_*.h"

y = N_VNew*(n,…);
cvmem = CVodeCreate(CV_BDF,CV_NEWTON);
flag = CVodeSet*(…);
flag = CVodeMalloc(cvmem,rhs,t0,y,…);
flag = CVSpgmr(cvmem,…);
yS = N_VNewVectorArray_*(Ns,…);
flag = CVodeSetSens*(…);
flag = CVodeSensMalloc(cvmem,…,yS);
for(tout = …) {
      flag = CVode(cvmem, …,y,…);
      flag = CVodeGetSens(cvmem,t,yS);
}
NV_Destroy(y);
NV_DestroyVectorArray(yS,Ns);
CVodeFree(&cvmem);
```

Adjoint Sensitivity Analysis in SUNDIALS

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```
#include “cvodes.h”
#include “cvodea.h”
#include “cvodes_spgmr.h”
#include “nvector_*.h”

y = N_VNew_*(n,…);
cvmem = CVodeCreate(CV_BDF,CV_NEWTON);
CVodeSet*(…);  CVodeMalloc(…);  CVSpgmr(…);

cvadj = CVadjMalloc(cvmem,STEPS);
flag = CVodeF(cvadj,…,&nchk);
yB = N_VNew_*(nB,…);
CVodeSet*B(…);  CVodeMallocB(…);  CVSpgmrB(…);
for(tout = …) {
      flag = CVodeB(cvadj, …,yB,…);
}

NV_Destroy(y);
NV_Destroy(yB);
CVodeFree(&cvmem);
CVadjFree(&cvadj);
```

Applications of SUNDIALS

- **Parallel CVODE is being used in a 3D tokamak turbulence model in LLNL's Magnetic Fusion Energy Division. A typical run has 7 unknowns on a 64x64x40 mesh, with up to 60 processors**
- **KINSOL with a HYPRE multigrid preconditioner is being applied within CASC to solve a nonlinear Richards' equation for pressure in porous media flows. Fully scalable performance was obtained on up to 225 processors on ASCI Blue.**
- **CVODE, KINSOL, IDA, with MG preconditioner, are being used to solve 3D neutral particle transport problems in CASC. Scalable performance obtained on up to 5800 processors on ASCI Red.**

Applications with sensitivity analysis

- SensPVODE, SensKINSOL, SensIDA used to determine solution sensitivities in neutral particle transport applications.
- IDA and SensIDA used in a cloud and aerosol microphysics model at LLNL to study cloud formation processes.
- SensKINSOL used for sensitivity analysis of groundwater simulations.
- CVODES used for sensitivity analysis of chemically reacting flows (SciDAC collaboration with Sandia Livermore).
- CVODES used for sensitivity analysis of radiation transport (diffusion approximation).
- KINSOL+CVODES used for inversion of large-scale time-dependent PDEs (atmospheric releases).

Influence of Opacity Parameters in Radiation-Diffusion Models

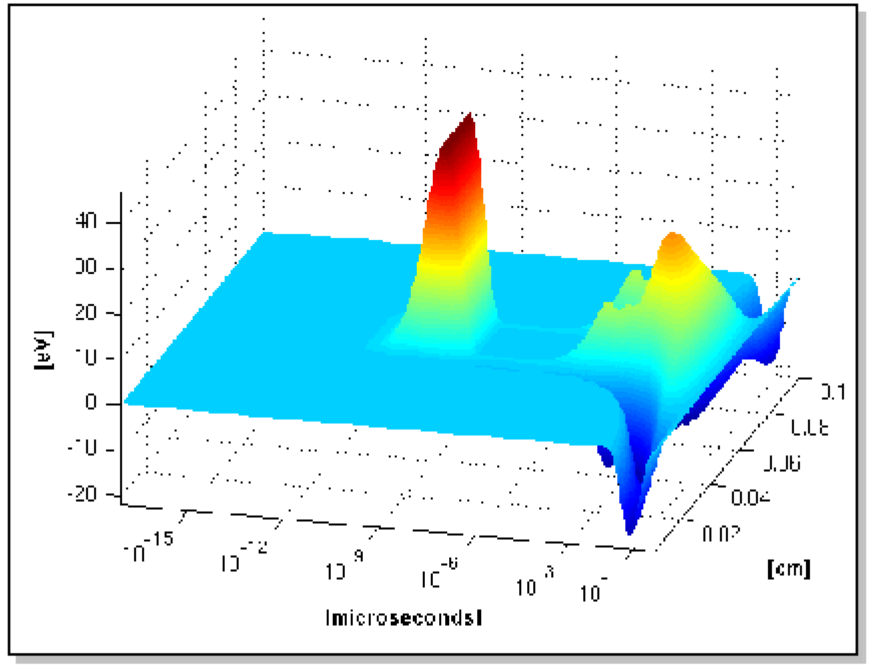
$$\frac{\partial E_R}{\partial t} = \nabla \cdot \left(\frac{c}{3\kappa_R(\rho, T_R) + \left\| \nabla E_R / E_R \right\|} \nabla E_R \right) + c\kappa_P(\rho, T_M)\left(aT_M^4 - E_R\right) + \chi(x) c a T_{source}^4$$

$$\frac{\partial E_M}{\partial t} = -c\kappa_P(\rho, T_M)\left(aT_M^4 - E_R\right)$$

- **Opacities and EOS are often given through look-up tables**
  Consider exponential opacities of the form

$$\kappa(\rho, T) = \omega \rho^\alpha T^\beta$$

- **Problem dimension: N_x = 100, N_p = 1**
- **Find sensitivities of temperatures w.r.t. opacity parameters (SensPVODE)**

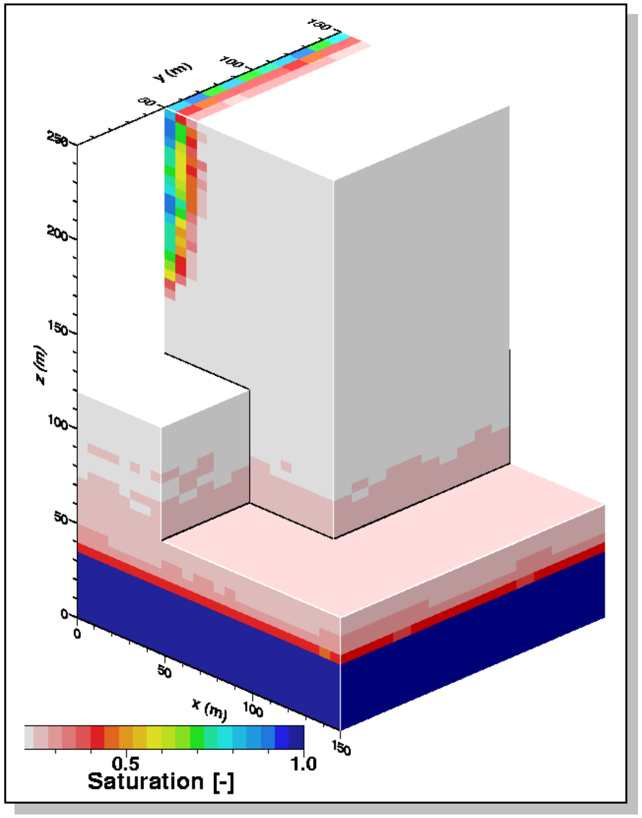


Scaled sensitivity of T_R w.r.t beta.
Early time effect of Plank opacity
Later effects of Rosseland opacity

Influence of Relative Permeability Parameters in Groundwater Simulation

$$\frac{\partial[s(p)\phi\rho]}{\partial t} - \nabla\cdot\left\{\frac{Kk_r(p)\rho}{\mu}(\nabla p - \rho g\nabla z)\right\} = q$$

$$k_r(p) = \frac{\left\{1-(\alpha|p|)^{n-1}\left[1+(\alpha|p|)^n\right]^{-m}\right\}^2}{\left[1+(\alpha|p|)^n\right]^{n/2}}$$

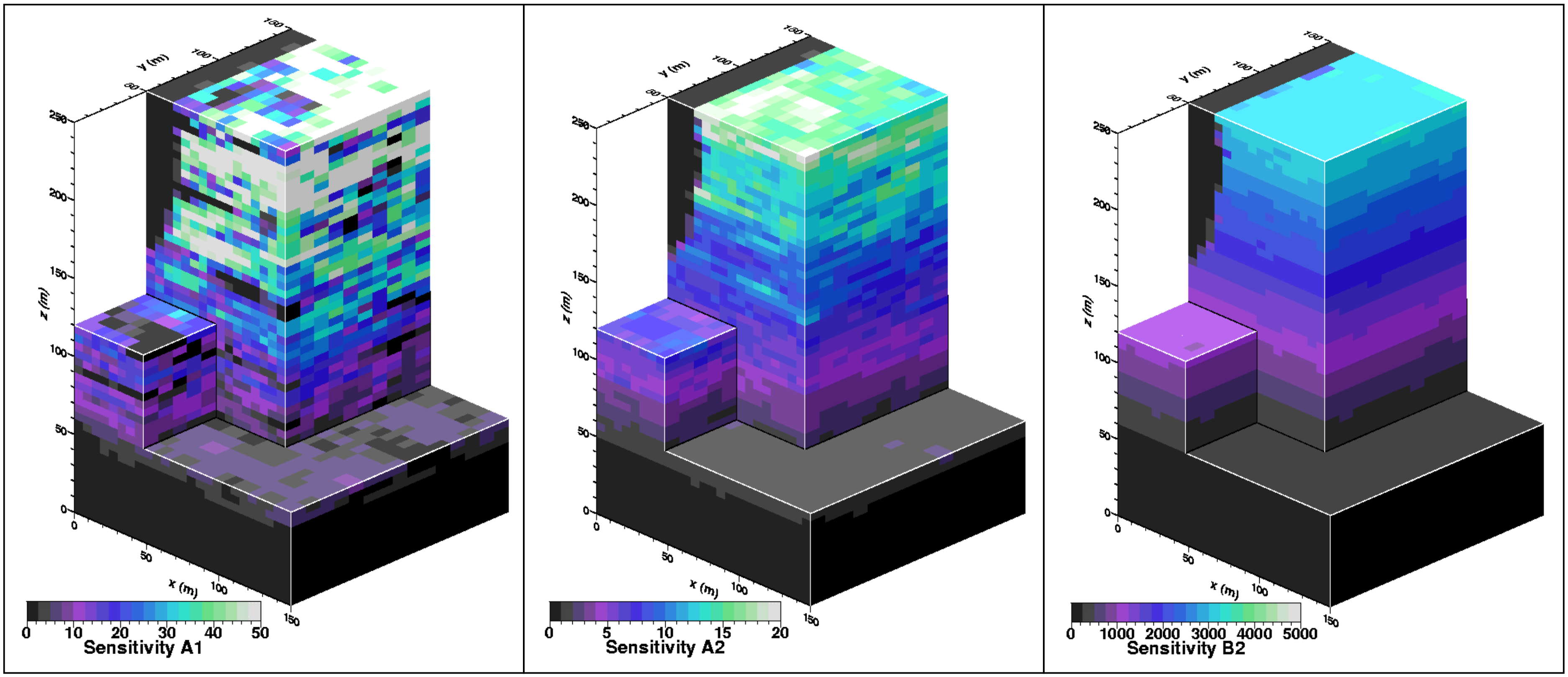


- **Sensitivity of water pressure to parameters in the expression for relative permeability:**

$$\alpha = a_1 \ln|K| + a_2$$
$$n = b_2$$

- **Problem dimension: N_x = 18750, N_p = 3**
- **Software: KINSOL and SensKINSOL**

Influence of Relative Permeability Parameters in Groundwater Simulation - Results



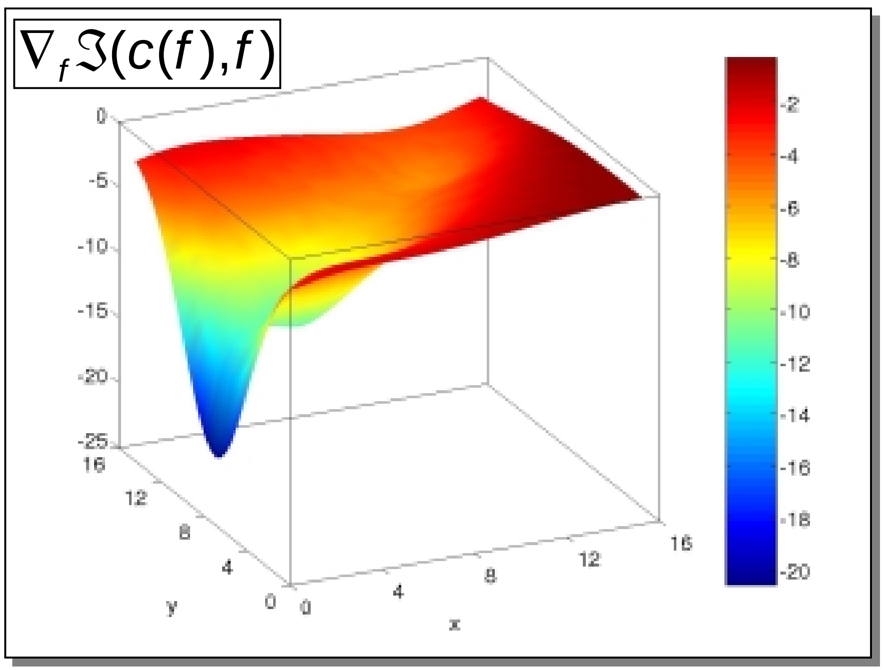
Sensitivity to a_1 | Sensitivity to a_2 | Sensitivity to b_2

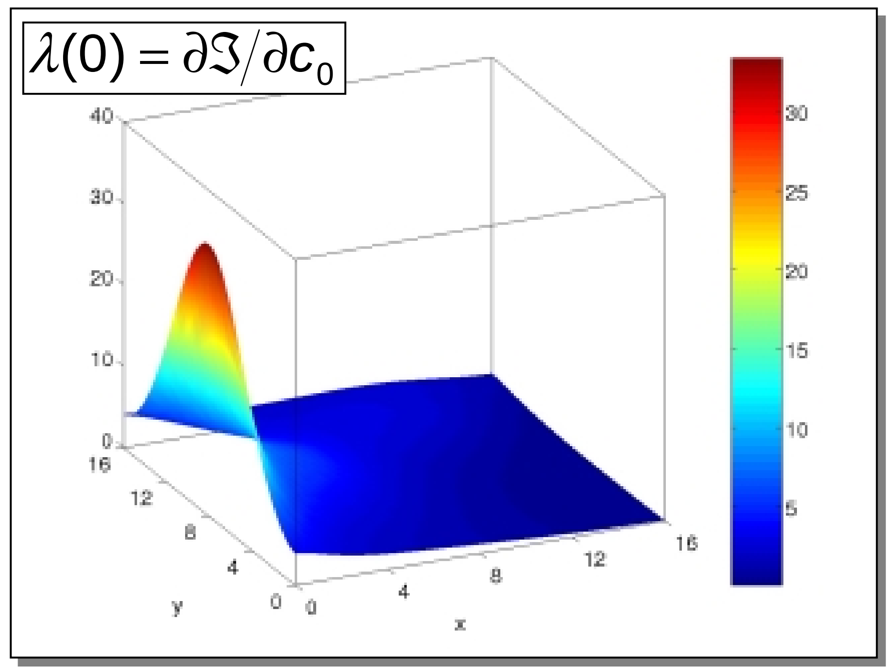
Atmospheric Event Reconstruction

$$\min_{f,c} \Im(c,f) := \frac{1}{2}\sum_{j=1}^{N_r}\int_t\int_\Omega \left(c - c^*\right)^2 \delta(x - x_j)\, d\Omega\, dt + \frac{1}{2}\beta R(f)$$

$$\begin{gathered} c_t - k\Delta c + \nabla c \cdot \vec{v} + f = 0,\ in\ \Omega \times (0,T) \\ \nabla c \cdot \vec{n} = 0,\ on\ \partial\Omega \times (0,T) \\ c = c_0(x),\ in\ \Omega\ at\ t = 0 \end{gathered}$$

$$\begin{gathered} -\lambda_t - k\Delta\lambda - \nabla\lambda \cdot \vec{v} = g(c,c^*),\ in\ \Omega \times (0,T) \\ \left(k\nabla\lambda + \lambda\vec{v}\right)\cdot\vec{n} = 0,\ on\ \partial\Omega \times (0,T) \\ \lambda(x) = 0,\ in\ \Omega\ at\ t = T \end{gathered}$$

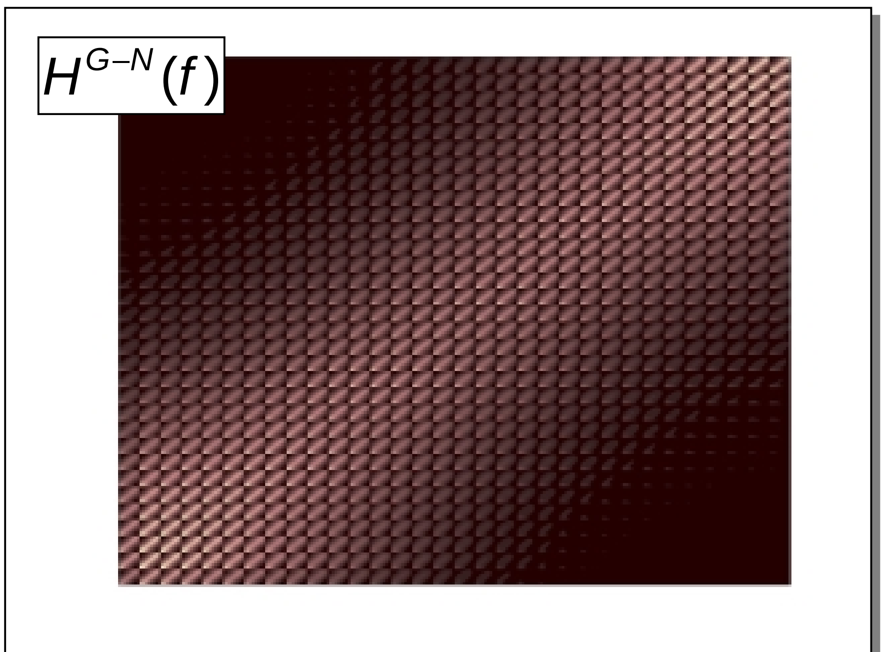


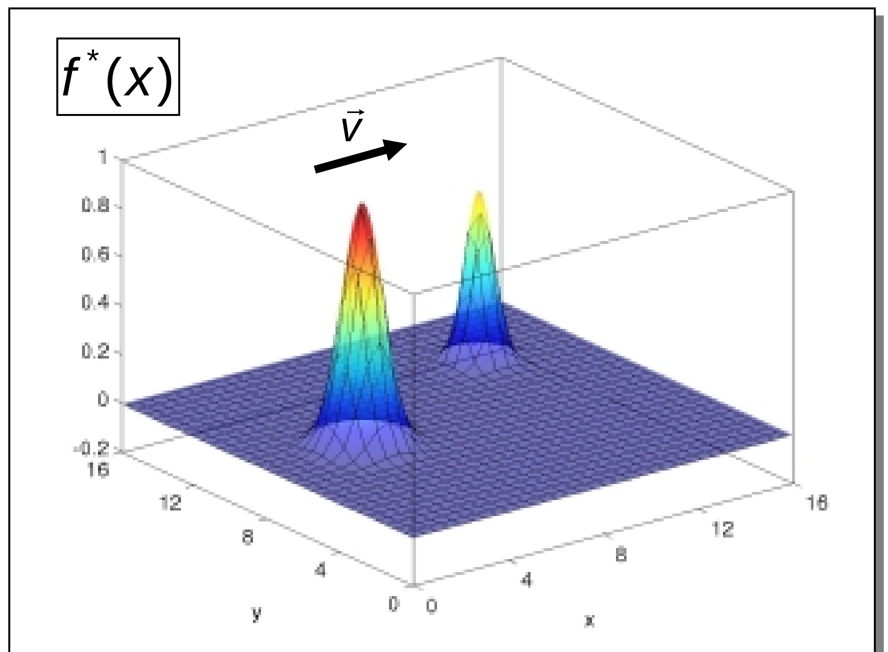


Atmospheric Event Reconstruction

- **CVODES – for gradient and Hessian-vector products**
- **KINSOL – for NLP solution**

- **Problem dimensions: N_{ODE}=4096, N_{NLP}=1024**





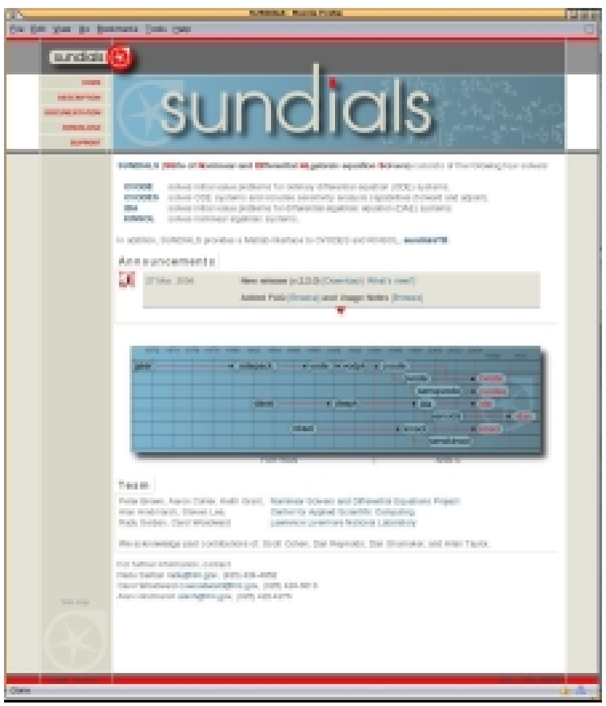
Current and Future Work

- IDAS (forward and adjoint sensitivity variant of IDA)
  - Early 2007
- Automatic generation of derivative information
  - Incorporation of AD tools (forward/reverse)
- Improved checkpointing / alternatives to checkpointing
  - Storage of integrator decision history

Availability

Open source BSD license
www.llnl.gov/CASC/sundials

Publications
www.llnl.gov/CASC/nsde



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Web site:

Individual codes download

SUNDIALS suite download

User manuals

User group email list

end

Forward Sensitivity Analysis

- **For a parameter dependent system**

$$\begin{cases} F(x,\dot{x},t,p) = 0 \\ x(0) = x_0(p) \end{cases}$$

find s_i=dx/dp_i by simultaneously solving the original system with the N_p sensitivity systems obtained by differentiating the original system with respect to each parameter in turn:

$$\boxed{\begin{cases} F_{\dot{x}}\dot{s}_i + F_x s_i + F_{p_i} = 0 \\ s_i(0) = dx_0 / dp_i \end{cases}, \quad i = 1,\ldots,N_p}$$

- **Gradient of a derived function** $g(t,x,p) \Rightarrow dg/dp = g_x s + g_p$
- **Obtain gradients with respect to p for any derived function**
- **Computational cost - $(1+N_p)N_x$ - increases with N_p**

Adjoint Sensitivity Analysis

- **index-0 and index-1 DAE**

$$\lambda^* F_{\dot{x}}\Big|_{t=T} = 0 \qquad \frac{dG}{dp} = \int_0^T (g_p - \lambda^* F_p)dt + (\lambda^* F_{\dot{x}})\Big|_{t=0} x_{0p}$$

- **Hessenberg index-2 DAE**

$$\begin{cases} \dot{x} = f^d(x,y,p) \\ 0 = f^a(x,p) \end{cases} \rightarrow \begin{cases} \dot{\lambda} + A^*\lambda + C^*\eta = -g_x^* \\ B^*\lambda = -g_y^* \end{cases}$$

$$A = \frac{\partial f^d}{\partial x}, B = \frac{\partial f^d}{\partial y}, C = \frac{\partial f^a}{\partial x}, \exists (CB)^{-1}$$

impose final conditions of the form $\lambda^*(T) = \xi^* C\Big|_{t=T}$

At $t = T$:

$$\lambda^* B = -g_y \Rightarrow \xi^* CB = -g_y \Rightarrow \xi^* = -g_y (CB)^{-1}$$
$$f^a(x,p) = 0 \Rightarrow Cx_p = -f_p^a \Rightarrow \lambda^* x_p = -\xi^* f_p^a$$

$$\lambda^*(T) = -g_y (CB)^{-1} C\Big|_{t=T} \qquad \frac{dG}{dp} = \int_0^T (g_p + \lambda^* f_p^d + \eta^* f_p^a)dt + \lambda^*(0)x_{0p} - g_y (CB)^{-1} f_p^a\Big|_{t=T}$$

$$\begin{cases} (\lambda^* F_{\dot{x}})' - \lambda^* F_x = -g_x \\ \lambda^* F_{\dot{x}} x_p = \ldots \quad \text{at } t = T \end{cases}$$

$$G(x,p) = \int_0^T g(t,x,p)dt$$

$$\frac{\mathrm{d}G}{\mathrm{d}p} = \int_0^T (g_p - \lambda^* F_p)dt - (\lambda^* F_{\dot{x}} x_p)\Big|_0^T$$